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Introduction

Mineral dust is a major Earth system component. Despite being the dominant aerosol by mass, global and regional dust **emission estimates** remain **highly uncertain** due to poorly constrained emission parameterizations. In this work, we aim to develop a **dust emission optimization framework**, combining **modern computational numerical modelling techniques** and **4D variational data assimilation algorithms**, to **improve dust emission estimates**.

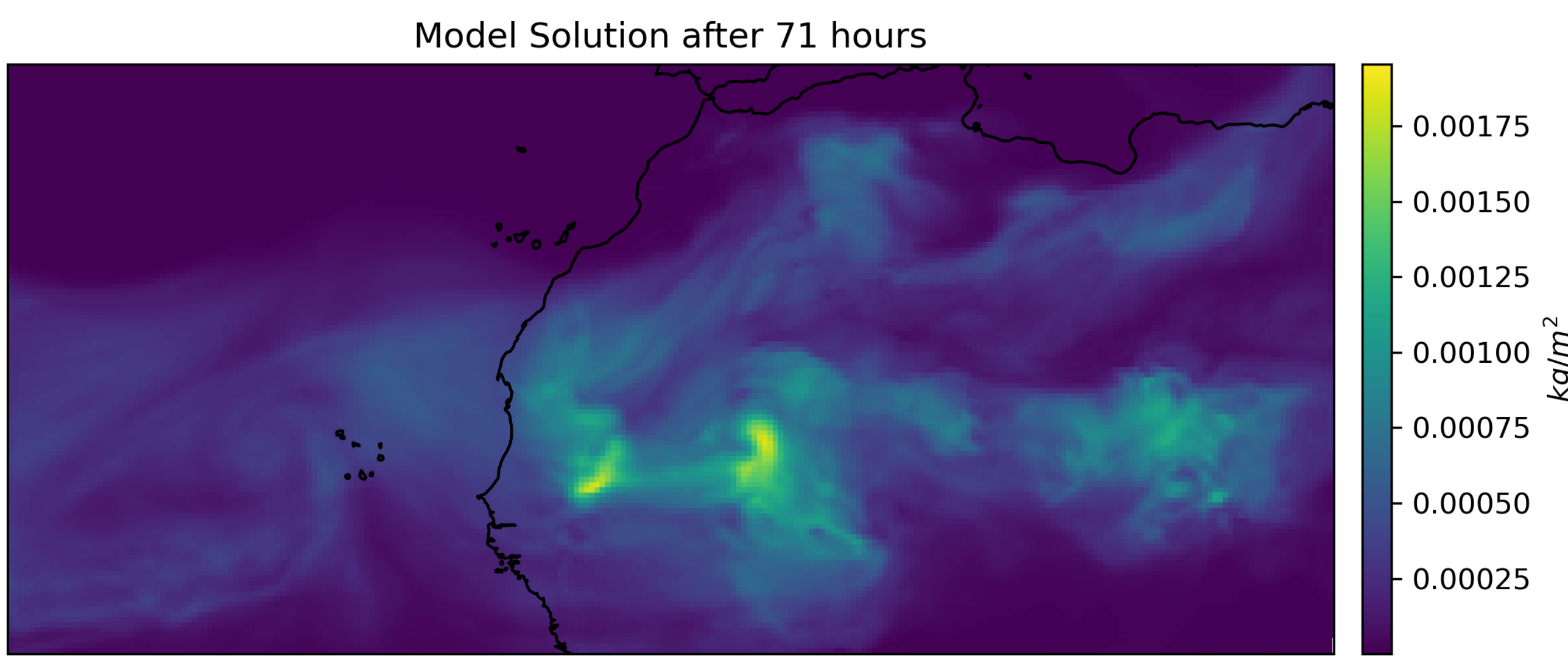
Python-JAX Dust Transport Model Description

We developed a **regional off-line** dust transport model, solving the dust mass continuity equation, entirely in **Python** using the **JAX** framework, enabling for:

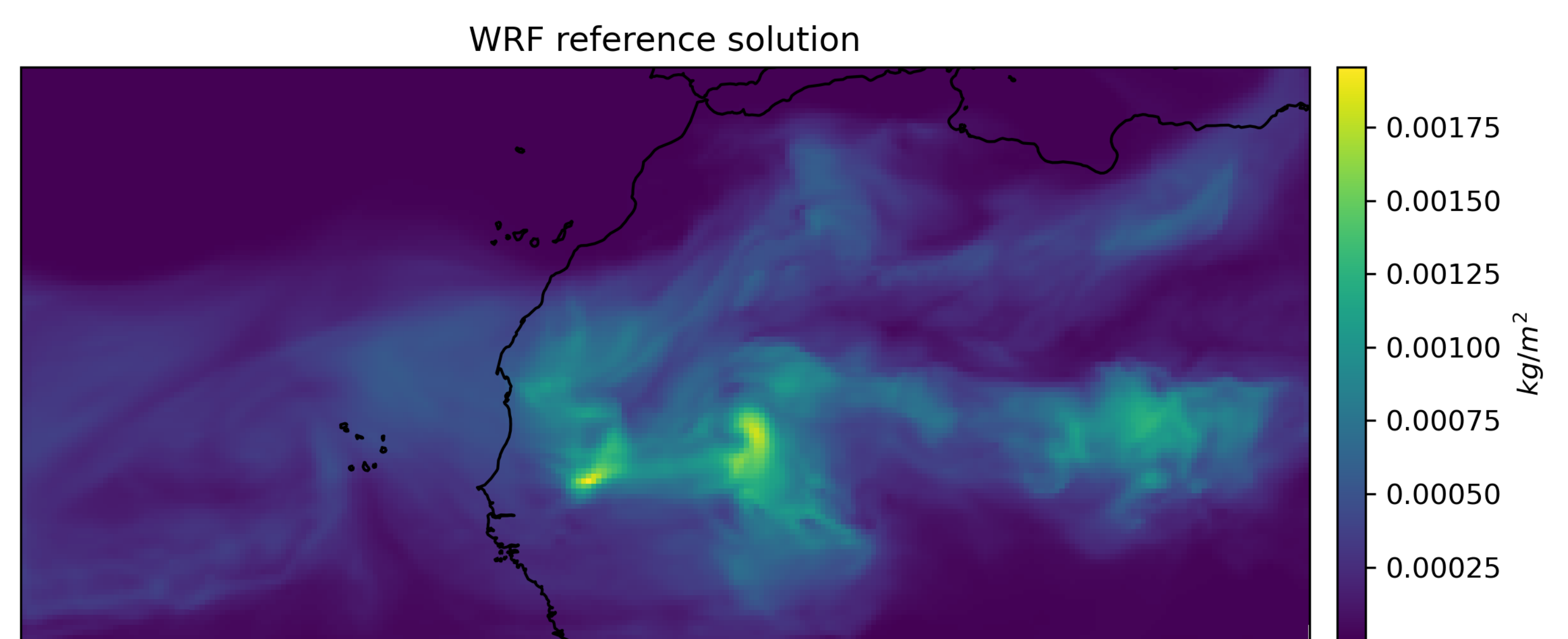
- **Just-in-Time (JIT)** compilation for **high computational efficiency**.
- **Hardware acceleration** and **parallel computation** on **CPUs/GPUs**.
- **Automatic differentiation** capabilities - **integration** with **variational data assimilation** and **machine-learning** workflows.

Numerical Schemes and parameterizations:

- **Advection:** Fifth-order horizontal, third-order vertical advection scheme in space, RK3 discretization in time, positive-definite flux limiter to preserve tracer positivity.
- **Diffusion:** Implicit diffusion solver.
- **Emission:** Ginoux et al (2001), Marticorena and Bergametti (1995).
- **Deposition:** Gravitational Settling (Stokes' law) and Resistance-based deposition approach (aerodynamic R_A and surface resistance R_S)



Total Column Dust (kg/m²) for Dust Bin 4, 71 hours simulation - Python-JAX transport model



Total Column Dust (kg/m²) for Dust Bin 4, 71 hours simulation - WRF reference

4D-Var Assimilation frameworks using JAX - Work in progress

Problem Formulation:

- Estimate **improved initial dust concentration** and **dust emission intensity fields**.
- **Incorporate** a spatially varying **2D tuning parameter a** into the dust emission scheme to scale emission fluxes.
- This leads to an **augmented state vector**: $x_0 = (q_0 \ a_0)^T$
- With **perturbations** and **adjoint variables**: $\delta x_0 = (\delta q_0 \ \delta a_0)^T$, $\lambda = (\lambda_q \ \lambda_a)^T$

Performing validation of TLM and Adjoint model:

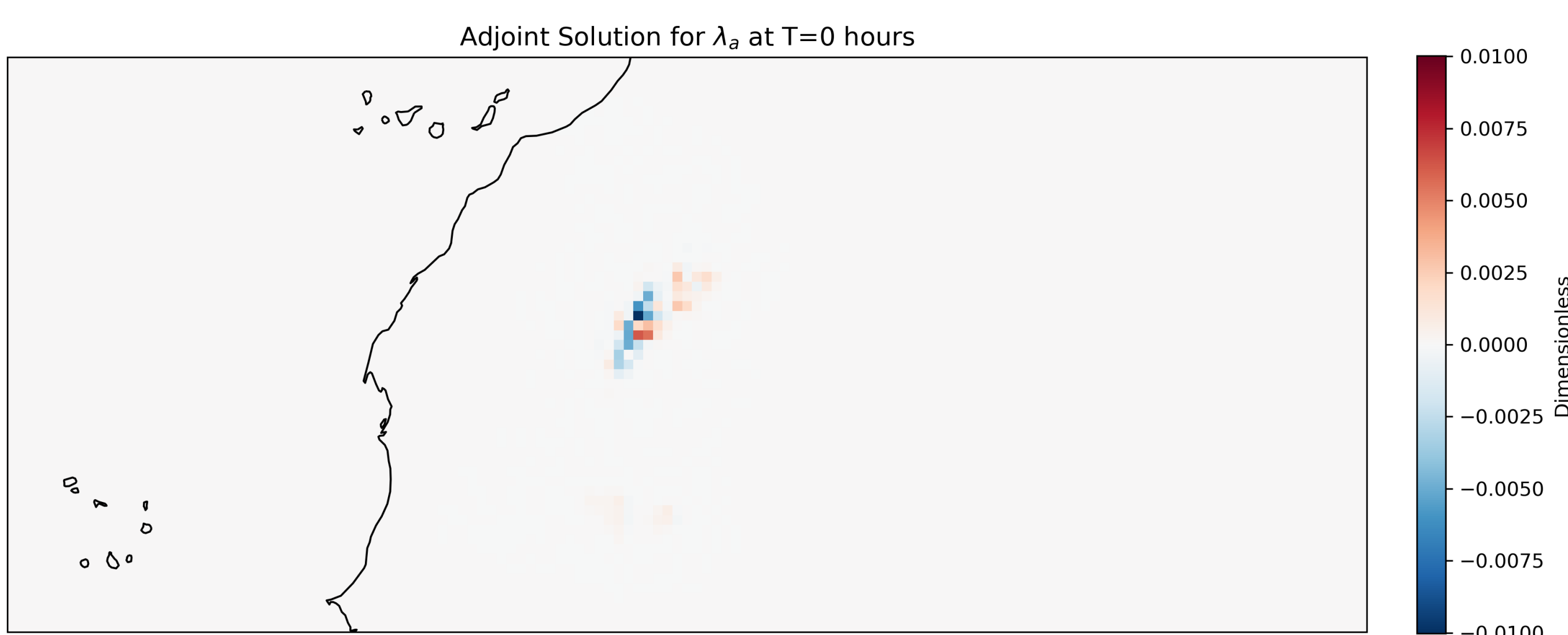
- The TLM validation uses a finite-perturbation consistency test:

$$\lim_{\epsilon \rightarrow 0} [M(x_0 + \epsilon \delta x) - M(x_0) - M(x_0)\epsilon \delta x] = 0$$

where M is the forward and M is the TLM.

- The Adjoint model M^T is validated using the definition:

$$\langle M\delta x, \lambda_T \rangle = \langle \delta x, M^T \lambda_T \rangle$$

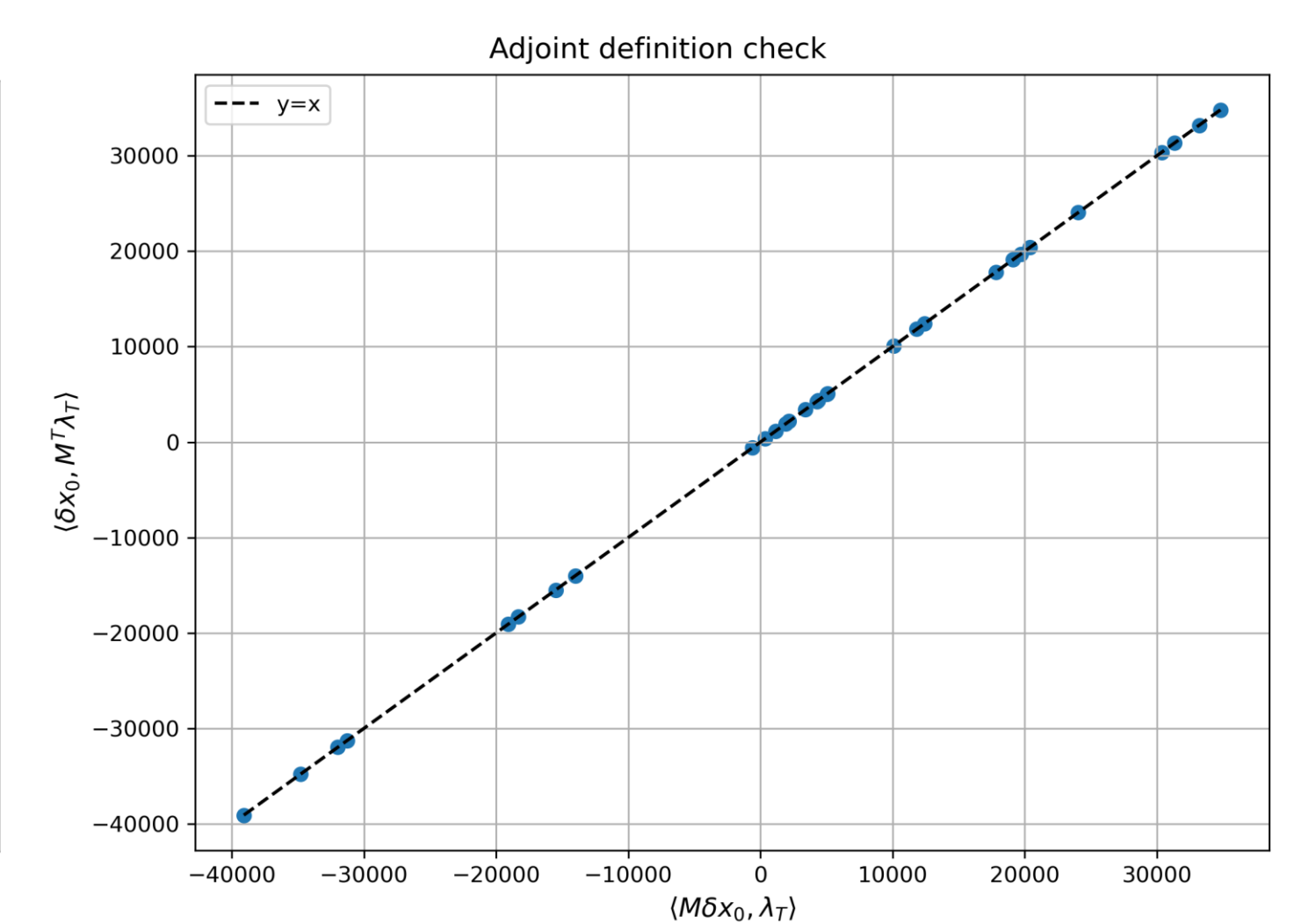
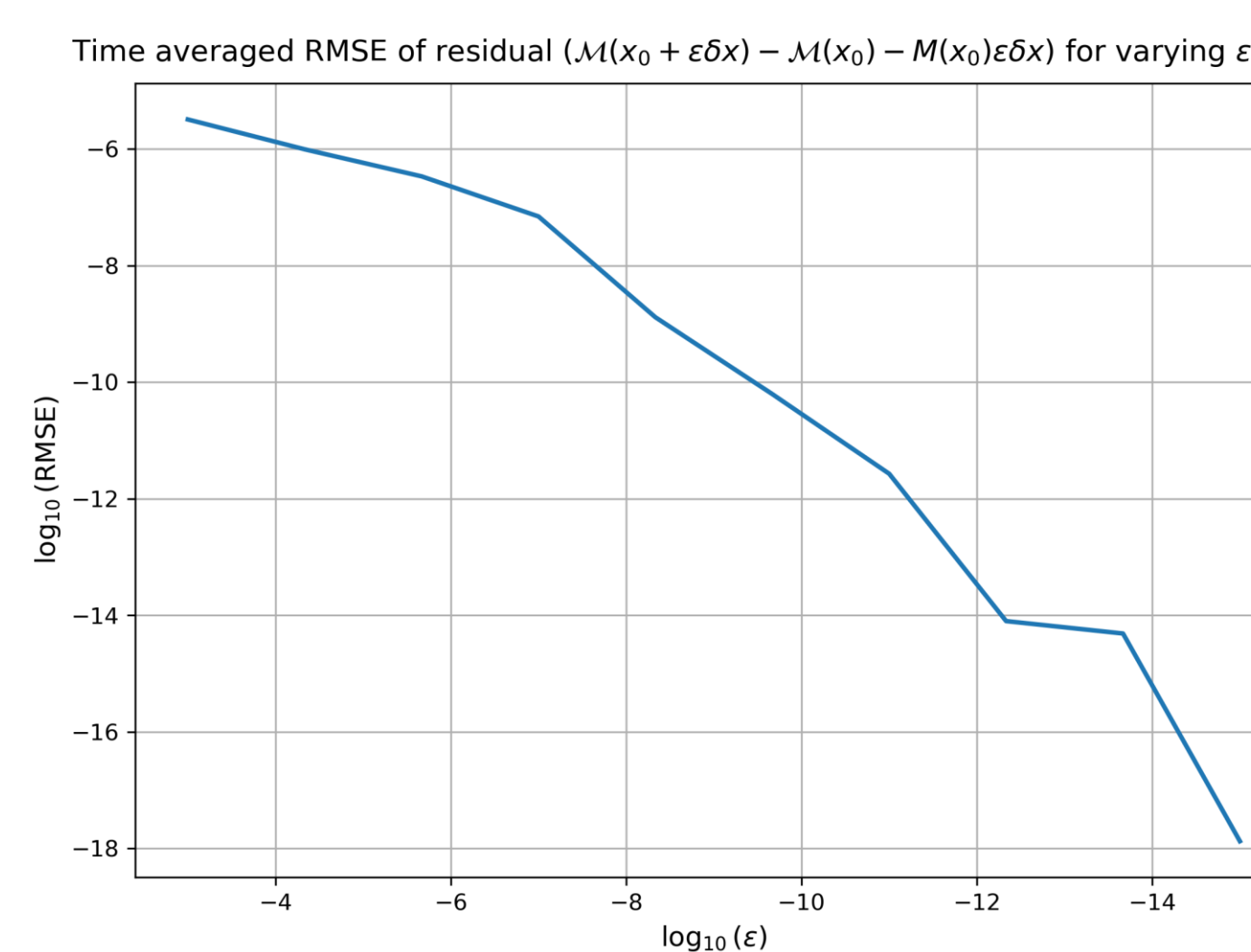


Adjoint model solution for variable λ_a at $t=0$, showing **sensitivity of the 2D tuning parameter a** to randomly generated synthetic «observations» of dust mass mixing ratio q .

Tangent Linear (TLM) and Adjoint models:

The JAX framework enables **automatic** construction (using **automatic differentiation** capabilities) directly from the forward model formulation using:

- Jacobian-vector product (**JVP**): $(x, u) \rightarrow \partial f(x)u$, propagating perturbations forward in time - **TLM**.
- Vector-Jacobian product (**VJP**), equivalent to: $(x, u) \rightarrow \partial f(x)^T u$ allowing sensitivity calculations - **Adjoint**.



Future work:

- Development of **4D-Var data assimilation frameworks**, including the **Strong-Constraint Incremental 4D-Var**, using the JAX-derived TLM and adjoint model
- **Assimilation of vertically resolved dust profiles** from **EarthCARE** products to better **constrain dust vertical distributions** and **emission intensity fields**.

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